
The NCEM Phase Extensions to Digital Micrograph

Roar Kilaas

User Manual

This package has been created by Dr. Roar Kilaas at the NCEM at the Lawrence Berkeley National Laboratory and Dr. Martin Hÿtch at CNRS, Vitry, France. The package is based largely on algorithms developed by Dr. Martin Hÿtch.

This work is supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

For communication on the routines, contact:

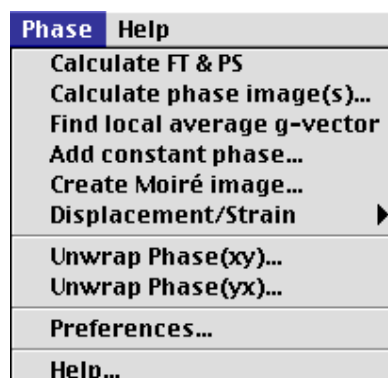
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For explanation on the concept of the geometric phase, see:

“Analysis of Variations in Structure from High Resolution Electron Microscope Images by Combining Real Space and Fourier Space information”, Martin J. Hÿtch, *Microsc. Microanal. Microstruct.* 8 (1997) 41-57

The NCEM Phase Extension Menu

The NCEM Phase Extension Menu



The package installs by placing the routines in the “Packages” folder that resides in the same location as the Digital Micrograph application. Once the program is started a new menu shows up in the menubar. The items in the menu are shown above and some of the menuitems point to sub-menus. The general operation of the various routines are described in the following sections.

Operating the routines

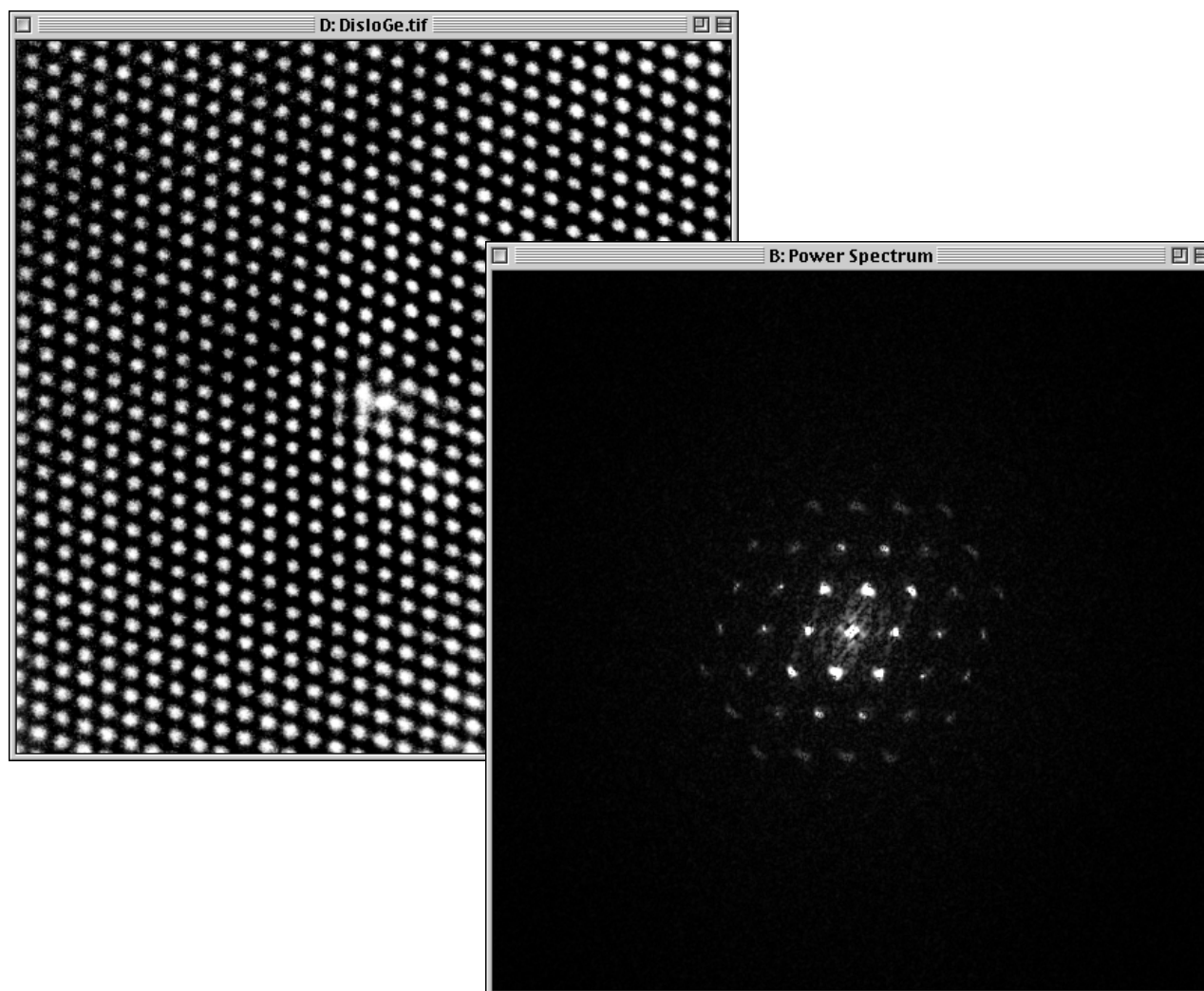
Calculate FT & PS....

Calculate FT & PS....

This is the beginning step of the procedure. You first need to calculate the Fourier Transform (*FT*) and the Power Spectrum (*PS*) of the image that you want to analyze. The Fourier Transform of the image is hidden and all the actual operations take place on the *FT* image. The *PS* is calculated using a Hanning window and is used for placing the selection which marks which vector **g** to use for calculating the corresponding phase/amplitude images. The only reason for doing this is that the *PS* image often shows better contrast than the *FT* and makes it easier to place the selection.

Many of the routines will be illustrated using an example of a HRTEM image of a dislocation in Germanium.

The images below show the HRTEM image (left) and the Power spectrum after invoking the “Calculate FT & PS...” command.



Note:

- 1) The image must be square and the dimensions must be powers of 2. Alternatively, a selection satisfying the criteria above must exist for the image to be analyzed.
- 2) The *FT* of the image is hidden and thus you may forget to delete it when starting the whole procedure over again for another image. If that is the case, the program complains that the FFT does not exist when it tries to create a phase image. This happens because you have

two images now called FFT and you will need to delete one of them (hopefully the right one).

- 3) You only need to do this first step once for each image you want to work on. You do not need to repeat this step when you want to work with another reflection. Just move the selection on the *PS* to the appropriate reflection.
- 4) In general if you get the message “Such and such image does not exist”, it will be either because you have two images of the same name, which happens if you use two reflections in succession and do not rename the first as “Phase Image 1” by using the menu-command Use as phase image #1 under displacement/strain or that you used the image as phase image 1/2 and then used an operation that still expected the phase image to be called “Phase Image”.

Create Phase Image

Create Phase Image

This routine calculates the geometric phase and other images associated with the chosen reflection.

The calculation performed is the inverse Fourier transform of the masked Fourier transform of the original image. The mask in question is a mask of the type defined below and centered on the reciprocal spatial frequency \mathbf{g} .

$$F^{-1}(\text{Masked } F(\text{Image})) \Rightarrow A(\mathbf{r})\exp\{2\pi i[\mathbf{g} \cdot \mathbf{r} + \partial\mathbf{g}(\mathbf{r}) \cdot \mathbf{r}]\} \\ A(r)\exp\{2\pi i[\mathbf{g} \cdot \mathbf{r} + \mathbf{g} \cdot \partial\mathbf{u}(\mathbf{r})]\}$$

giving rise to an

amplitude image $A(\mathbf{r})$

and a

phase image $P(\mathbf{r}) = -2\pi\mathbf{g} \cdot \partial\mathbf{u}(\mathbf{r})$

The term $2\pi\mathbf{g} \cdot \mathbf{r}$ has been subtracted from the phase, which is equivalent to moving the origin to the position of the reflection \mathbf{g} .

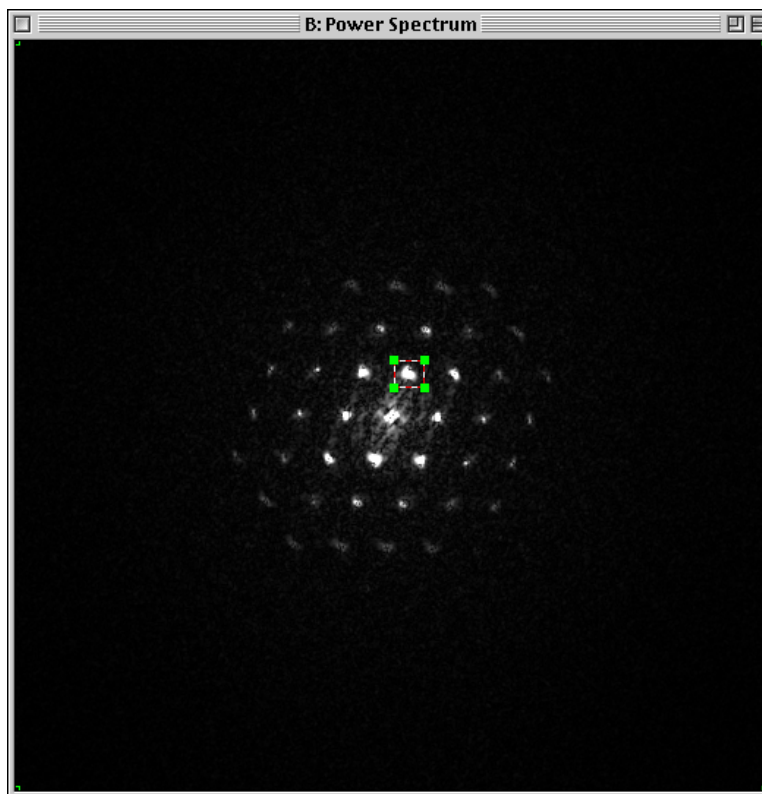
$\partial\mathbf{u}(\mathbf{r})$ is the displacement field with respect to the lattice planes defined by the frequency \mathbf{g} .

For calculating the local value of everywhere, this is done as:

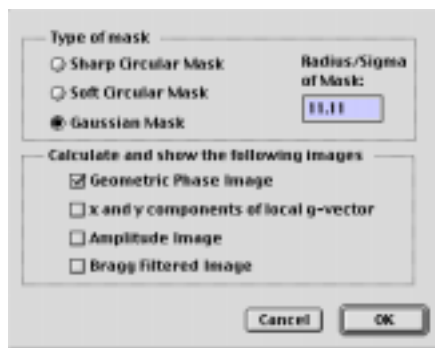
$$\mathbf{g}(\mathbf{r}) = -\partial/\partial\mathbf{r} P(\mathbf{r}) + \mathbf{g}$$

Usage:

- 1) A selection using the selection tool must first be made around a vector \mathbf{g} to use for determining the phase.



- 2) Invoke the menu command Calculate Phase Image(s)...
- 3) A dialog will give you the options available or creating the phase image.



Options:

Mask

The following choices to the type of mask can be made

- A sharp circular mask,
 $M = 1, r \leq R, M = 0, r > R$
- A soft circular mask, using a Gaussian edge
with a halfwidth of 1/5 of the radius
 $M = 1, r < 0.8R;$
 $M = \exp\{- (r-0.8R)^2/\sigma^2\}$
for $r \geq 0.8R, \sigma = 0.2R$
- A Gaussian mask, $\exp(-r^2/\sigma^2)$

Output

- Keep the geometric phase image(default). Normally this is what you want.
- Calculate and display the local **g**-vector.
- This calculates two images containing the x and y components of **g(r)** at each point in the image.
- Keep and display the amplitude image.
- Keep and display the masked **FT** from which the amplitude and phase images are calculated.

The resulting phase image is calculated by subtracting out the term

$$P_0 = 2\pi \mathbf{g}_0 \cdot \mathbf{r}$$

where \mathbf{g}_0 is given by the value returned from finding the position for the peak intensity in the power spectrum.

The resulting images are by default named Phase Image & Amplitude Image



Note:

- 1) After the phase image is calculated the next operation is to refine the local \mathbf{g} vector. This is performed by selecting an area in the phase image over which the lattice spacing are considered constant and invoking the menu-command Find local average \mathbf{g} -vector. This implies that the spacings found this way becomes a reference to which subsequent calculations are related.
- 2) Before calculating a phase image for another non-colinear frequency \mathbf{g}_2 for use in calculating local lattice spacings or displacements/strain, one should use the option “Use as Phase Image #1” for setting the \mathbf{g} used in this calculation to \mathbf{g}_1 which automatically renames the image “Phase Image” to “Phase Image 1”.

- 3) After having set the first phase image to “Phase Image 1”, the next step would be to move the selection on the **PS** to another reflection and using the command “Calculate Phase Image(s)” over again, refining the local vector for the same area and then setting the image as “Phase Image 2” before calculating displacements or strain.

For the second phase image one would then choose “Use as Phase image #2”.

Refine local g-vector

Refine local g-vector

Background :

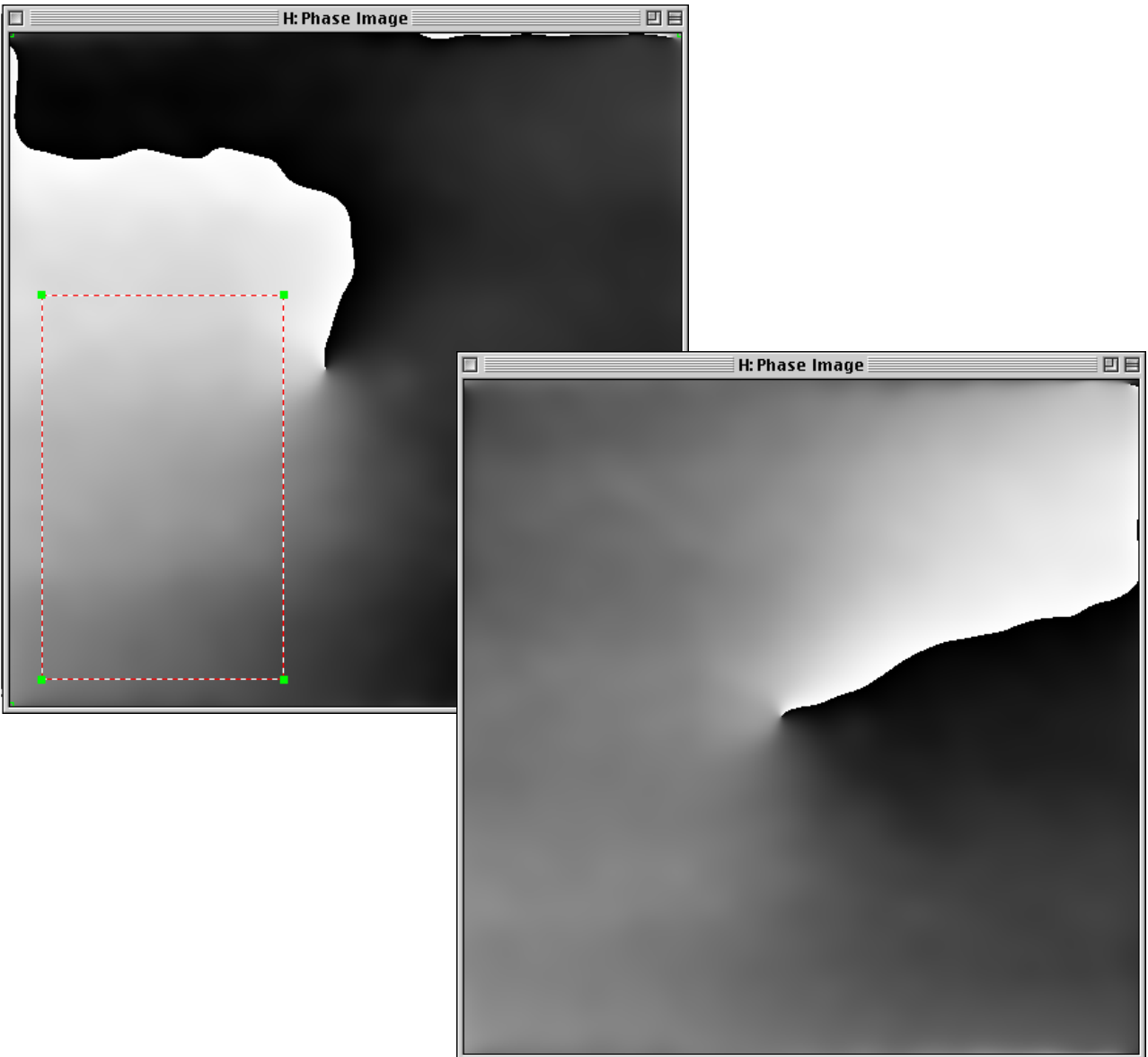
In order to calculate displacements or strain one needs a reference lattice. The vector **g** that is found when creating the phase image in the previous command is the one with the highest amplitude and is not necessarily the one that one would like to choose for the reference lattice. In order to further refine the vector **g** one chooses an area with the selection tool that is the area that is to become the reference area from which to calculate an average lattice-spacing. In order to define a reference lattice one needs two vectors **g**₁ and **g**₂ which both will need to be refined with respect to the same area.

Usage :

Mark an area with the selection tool where you want to find the average **g**-vector.

Run the command “Find local average g-vector”. The command will determine if there is a residual ramp $2\pi\partial\mathbf{g}\cdot\mathbf{r}$ within the selected area that should be subtracted out. The correction $\partial\mathbf{g}$ is added to the vector **g** that was found during “Calculate phase image(s)”. The routine can be used iteratively to refine the vector **g**, by using successively larger selections if the first selection needs to be small because of phase-jumps.

The images below show the original phase image with a selection marking



the area which will be used to find the average local g-vector. To the right, is displayed the result of the operation.

Note :

As mentioned above, two vectors \mathbf{g}_1 and \mathbf{g}_2 are used for defining a reference lattice. Thus normally this command is used for each vector \mathbf{g} from which a phase image is calculated before the phase image is referred to as phase image #1,2.

Add Phase

Add Phase

This routine adds a constant phase to the image “Phase Image”. Under normal operation this command is not used. It can be used to remove discontinuities associated with wrap around effects as the phase crosses 2π

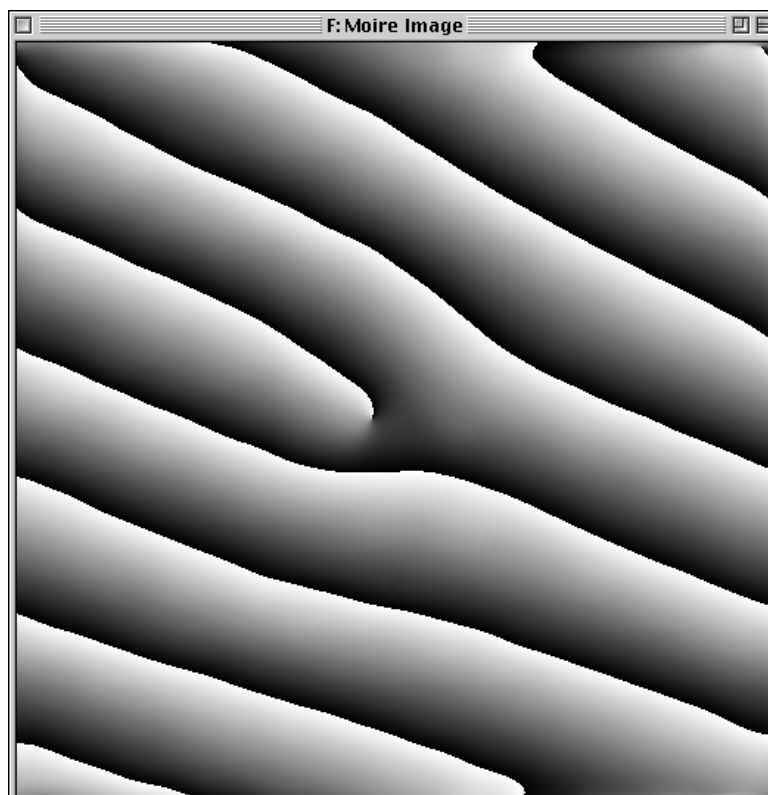
Create Moiré

Create Moiré

Usage :

Use this routine to create a Moiré image calculated from the image “Phase Image”. It is equivalent to moving the origin for the reciprocal space inverse FFT to the point $|\mathbf{g}|/M$ along the line from the origin to the spatial frequency \mathbf{g} . Mathematically, the Moiré image becomes

$P(\mathbf{r}) = 2\pi\mathbf{g} \cdot \mathbf{r}/M - 2\pi\mathbf{g} \cdot \partial\mathbf{u}(\mathbf{r})$ where M is the magnification chosen in the dialog box.



$M \rightarrow \infty$ gives the geometric phase image calculated in the “Calculate phase image(s)” command.

Displacement / Strain

Displacement / Strain

Displacement/Strain ▶	Use As Phase Image #1
Unwrap Phase(xy)...	Use As Phase Image #2
Unwrap Phase(yx)...	Calculate Displacements...
Preferences...	Calculate Strain...
	Calculate Local Lattice...

Use As Phase Image # 1

Use As Phase Image # 1

This command takes the **g**-vector associated with the image “Phase Image” and stores the values as the components (g_{1x}, g_{1y}) of the vector \mathbf{g}_1 . It defines a set of reference planes for further analysis. It also renames the image “Phase Image” to “Phase Image 1”. Use this command before you change the selection on the Power Spectrum to refer to a new **g**-vector.

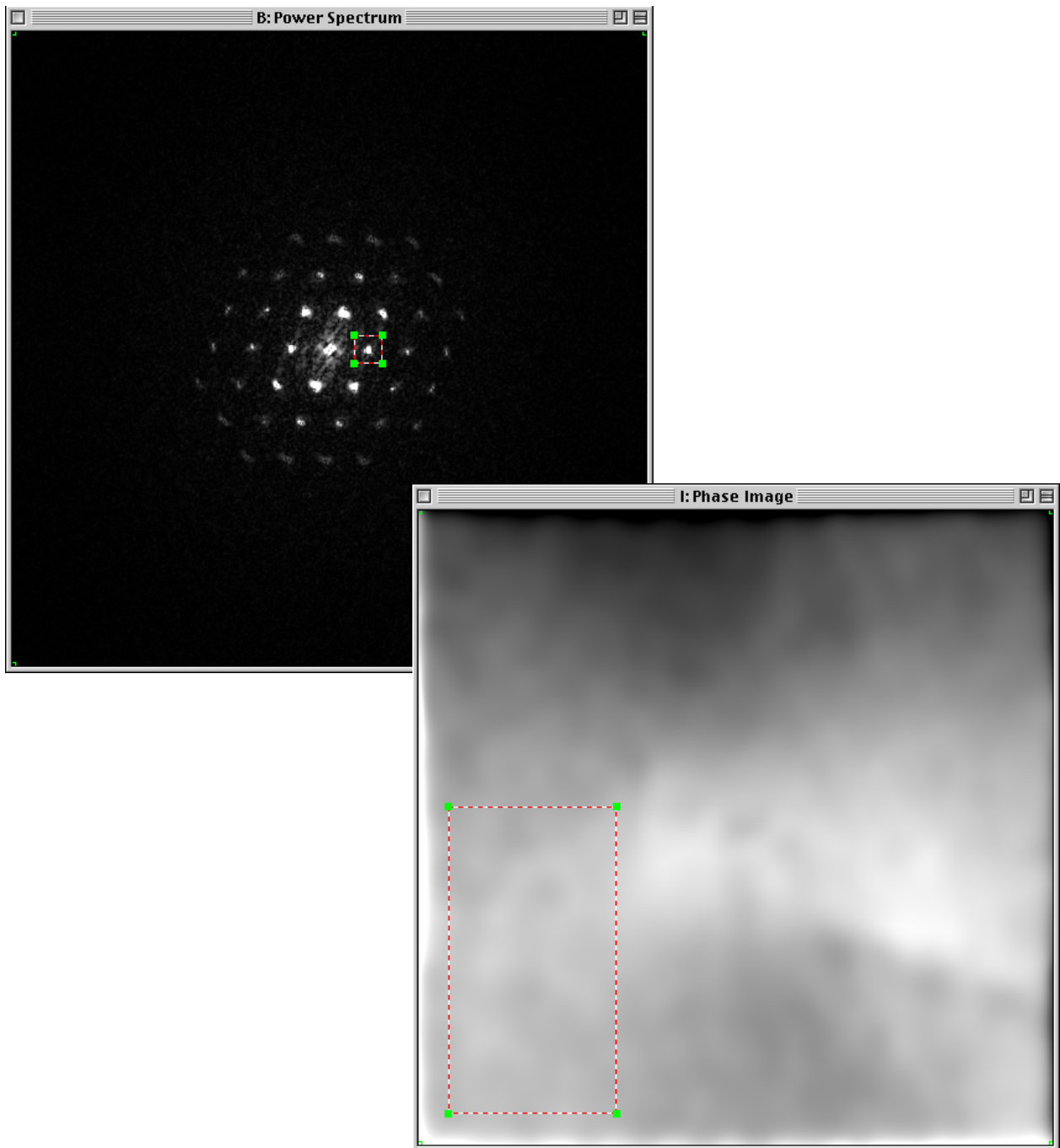
Use As Phase Image # 2

Use As Phase Image # 2

This command takes the **g**-vector associated with the image “Phase Image” and stores the values as the components (g_{2x}, g_{2y}) of the vector \mathbf{g}_2 . It defines a set of reference planes for further analysis. It also renames the image “Phase Image” to “Phase Image 2”. Use this command after you have defined “Phase Image 1” and \mathbf{g}_2 (g_{1x}, g_{1y}).

The two vectors $\mathbf{g}_1(g_{1x}, g_{1y})$ and $\mathbf{g}_2(g_{2x}, g_{2y})$ define a reference lattice (unit cell) for further analysis.

The left image below shows the power spectrum with the reflection to be



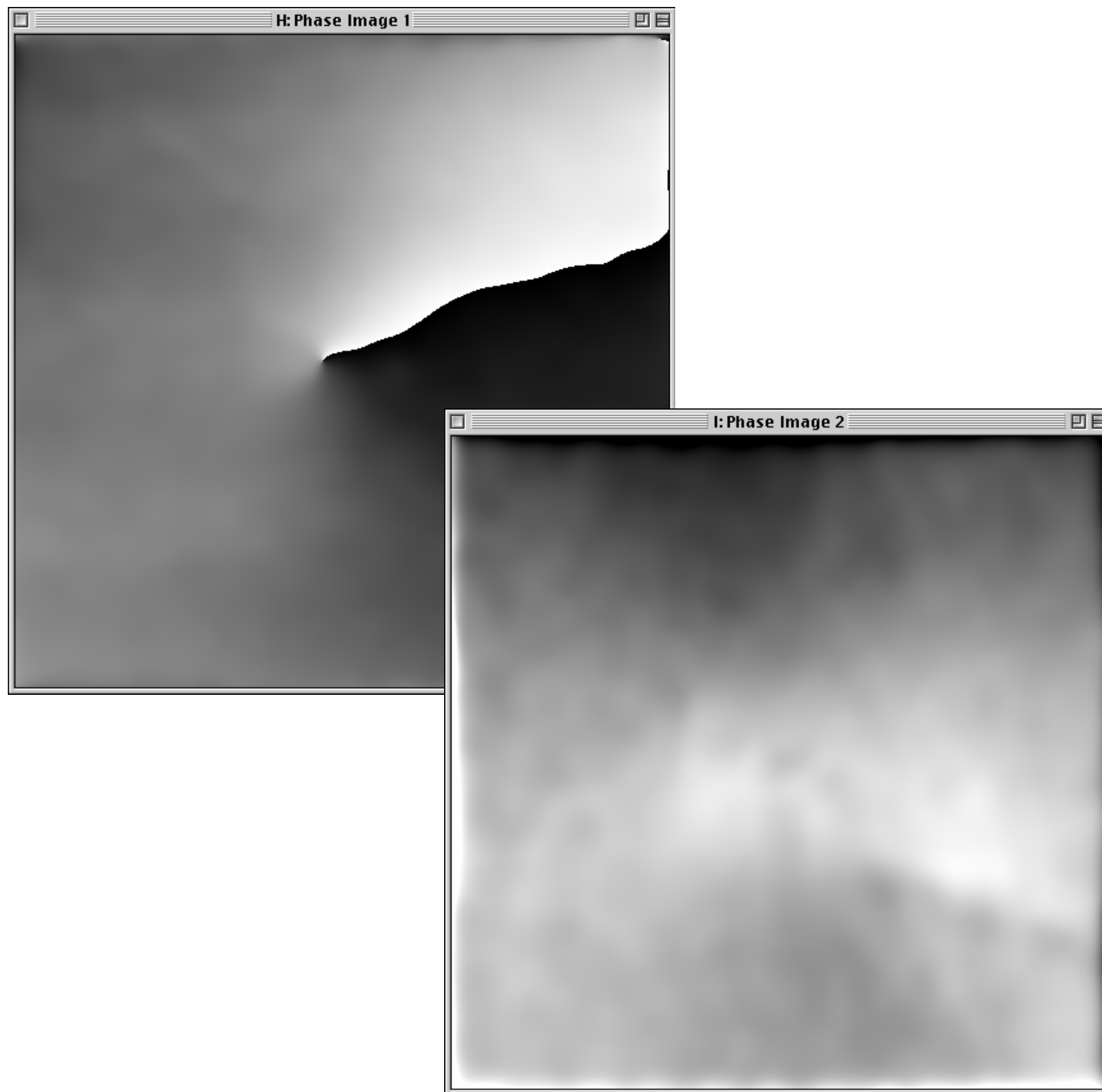
used as g-vector 2 and the right image shows the corresponding phase image after refining for the local lattice vector over the region shown in the selection.

Calculate Displacements

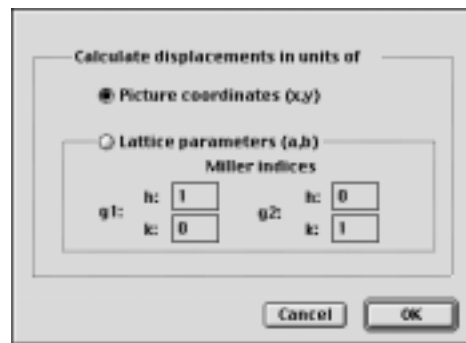
Calculate Displacements

Executing this command produces two images u_x and u_y which are the local x,y displacements with respect to the lattice defined by \mathbf{g}_1 & \mathbf{g}_2 .

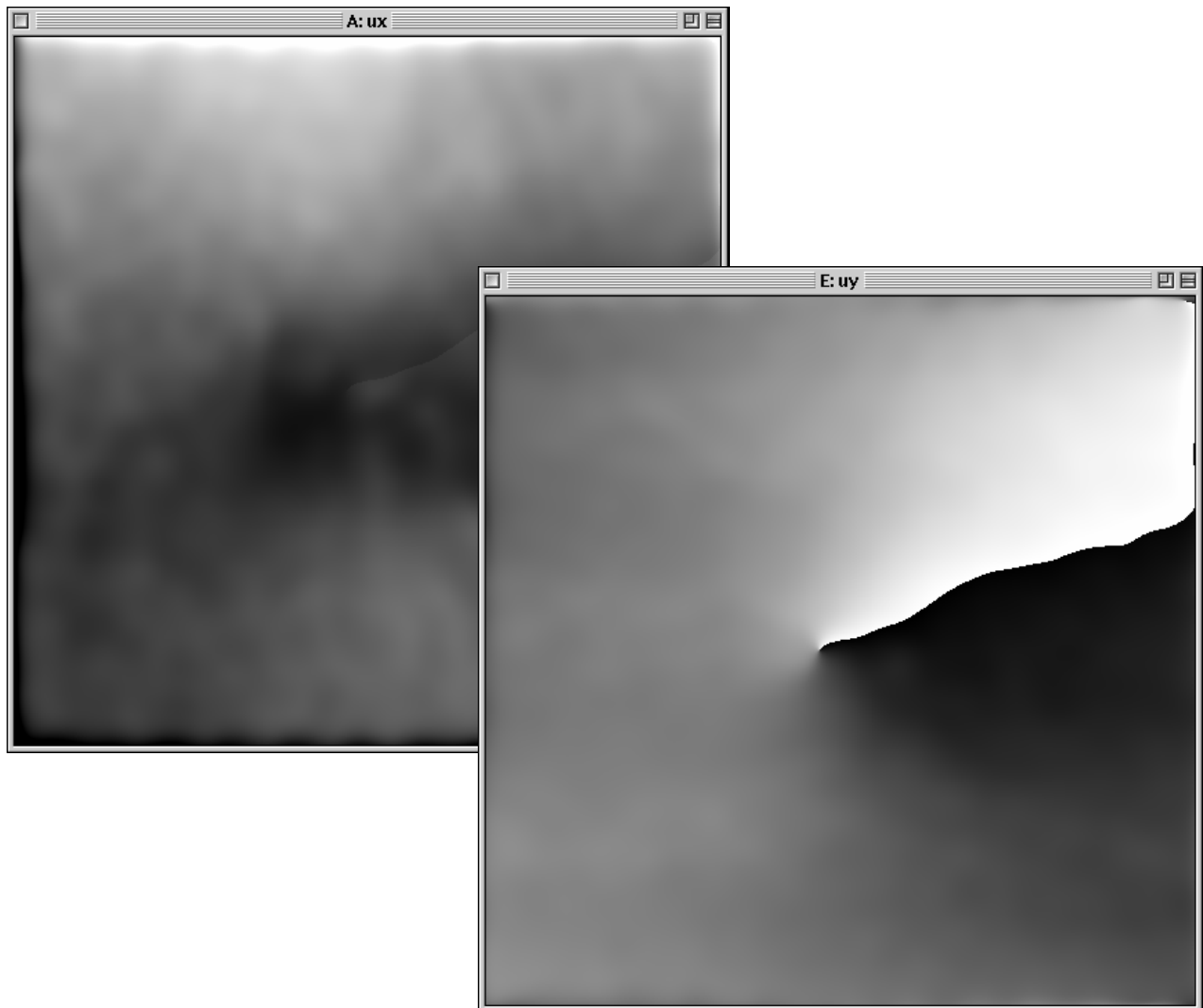
The command requires that the two images “Phase Image 1” and “Phase Image 2” exist together with the associated values for \mathbf{g}_1 and \mathbf{g}_2 .



Invoking the command brings up the following dialog box.



producing the following output as the result of the operation.

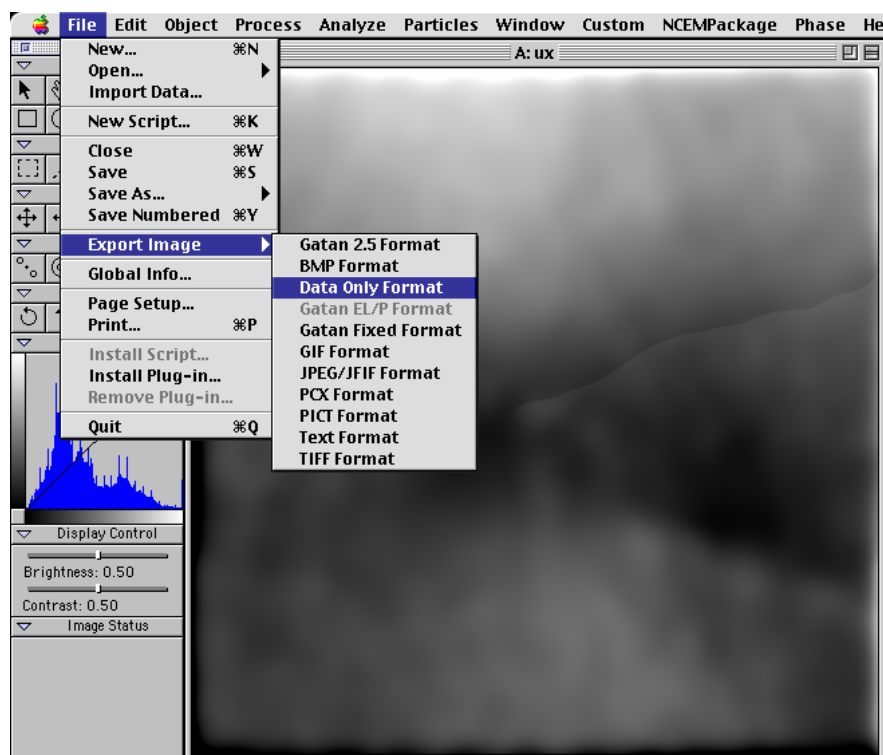


Prerequisite:

Both g_1 and g_2 including the associated images “Phase Image 1” & “Phase Image 2” must exist prior to executing this command.

Note:

Digital Micrograph currently has no capability of displaying the displacements as a vector plot. At the NCEM the X/Y-Displacements are saved as “Data Only” files and the program “Spyglass Transform” is used to read the data back in to display the displacements pictorially.



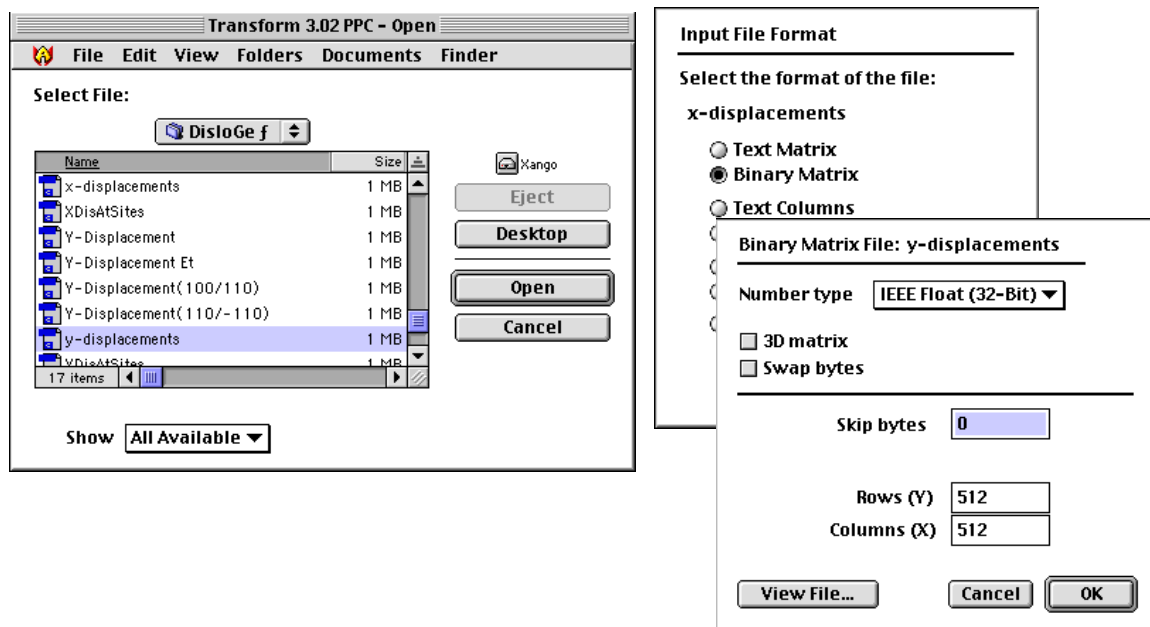
The files that are produced are binary files of type real 4 with the dimensions given by the size of the original image.

The following section demonstrates how the program Spyglass Transform may be used to display the data for the displacements.

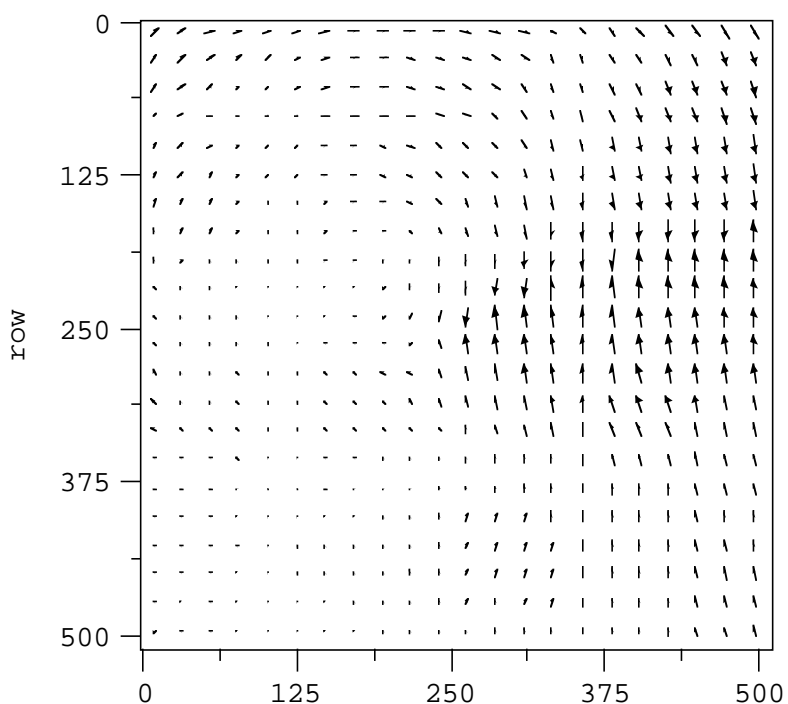
The user is free to represent the displacements in any form he/she chooses.

The first step is to open the files from within Spyglass Transform and fill in the required data so that the program knows how to interpret the file.

Calculate Displacements

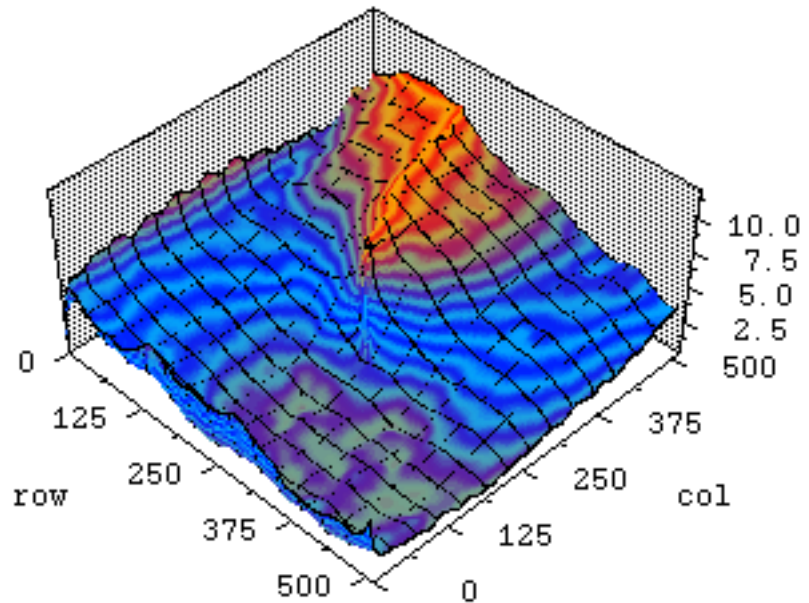


Below is shown a vector plot using the x-displacements as the length of the

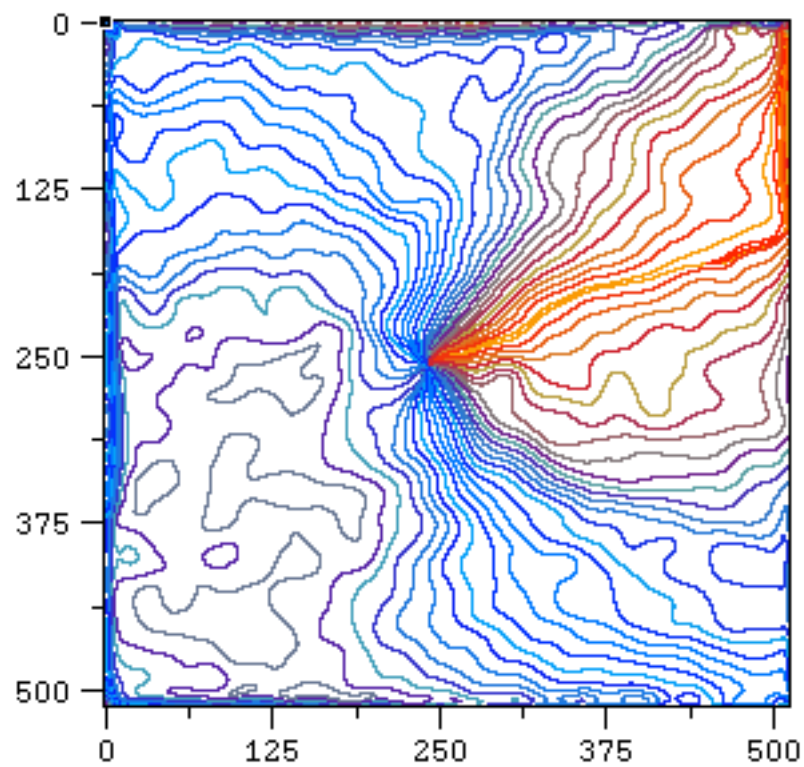


x-component of the vector and the y-displacement as the y-component of the vector.

The data can also be shown as a surface plot depicting the magnitude of the displacement.



Alternatively the magnitude of the displacement can be shown as a contour map as illustrated below.



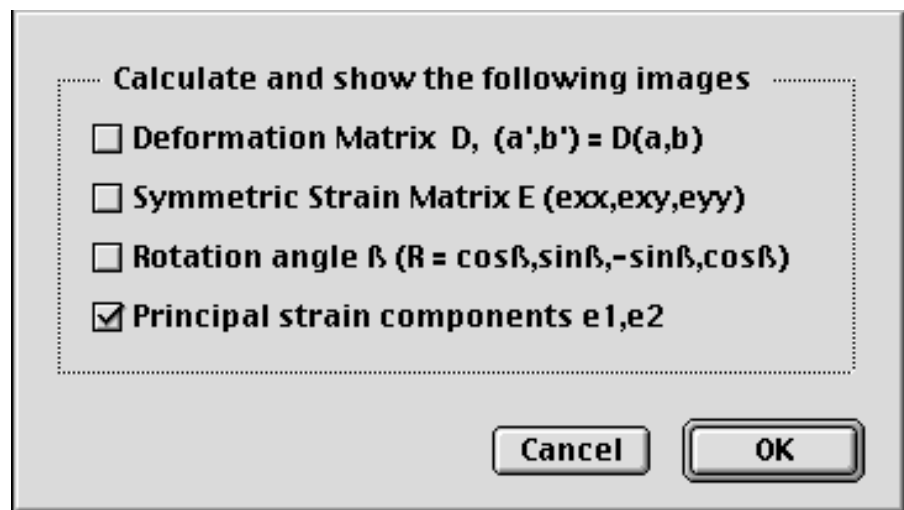
Calculate Strain

Calculate Strain

This command calculates the strain with respect to the reference lattice defined by \mathbf{g}_1 & \mathbf{g}_2 .

Prerequisite:

The two phase images “Phase Image 1” and “Phase Image 2” must have been calculated.

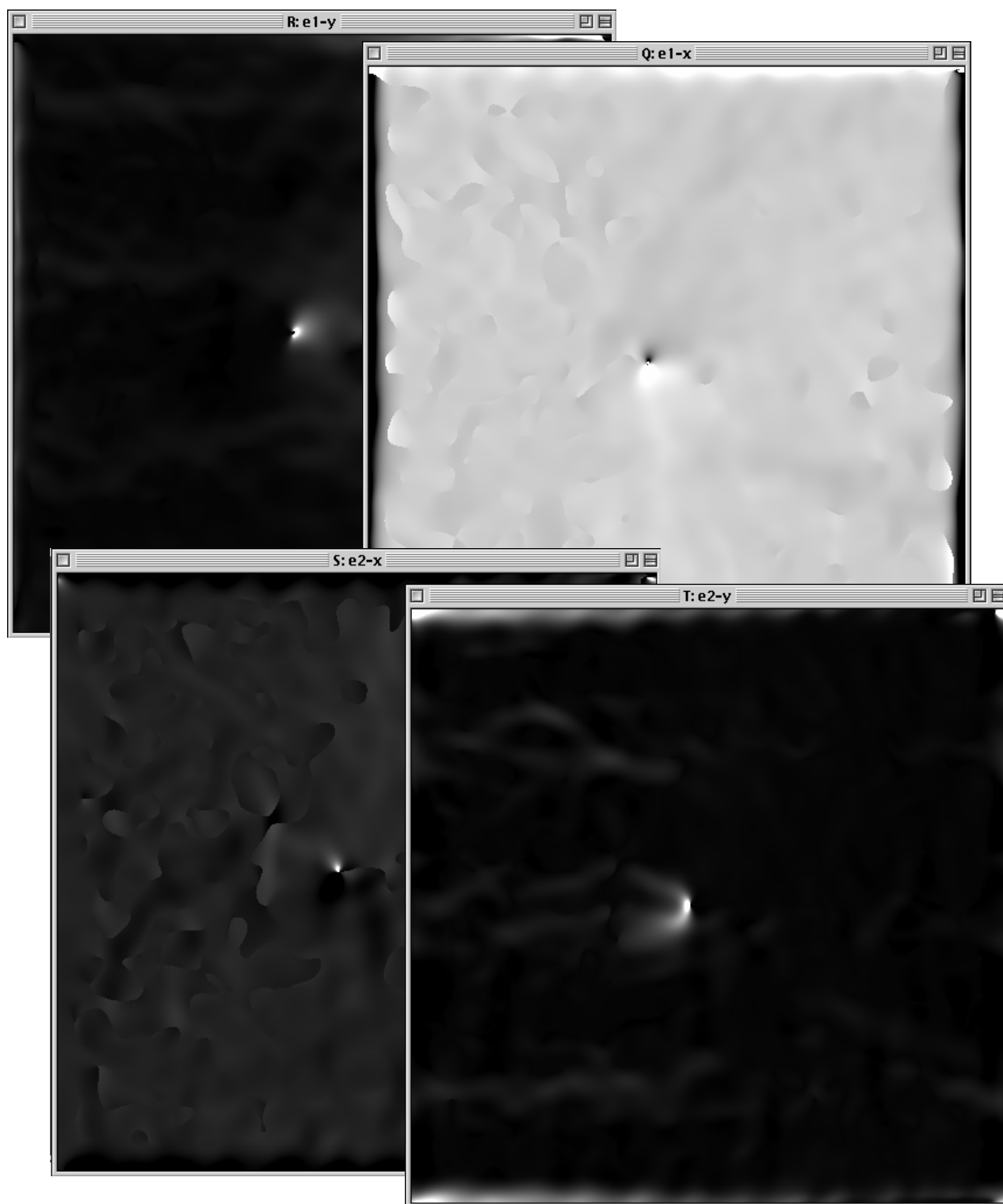


Results:

Depending on the requested output, the result will be one or more of the following

- a) the Deformation Matrix
- b) the Symmetric Strain Matrix
- c) the Rotation Angle
- d) the Principal Strain Components

The images on the next page illustrate the output produced by choosing to calculate and display the principal strain components e_1 and e_2 . Four images are produced, the x and y components of e_1 and the x and y components of e_2 .



Procedure:

The program first calculates the deformation matrix

$$D = \begin{bmatrix} e_{xx} & e_{xy} \\ e_{yx} & e_{yy} \end{bmatrix}$$

which relates the positions of a point \mathbf{r}' (x',y') to its unstrained location \mathbf{r} (x,y) through the relationship

$$\mathbf{r}' = (1+D)\mathbf{r} = S\mathbf{r}$$

The matrix S is then decomposed into a symmetric matrix S' and a rotation matrix W

$$S = \begin{bmatrix} 1 + e'_{xx} & e'_{xy} \\ e'_{yx} & 1 + e'_{yy} \end{bmatrix}$$

and

$$W = \begin{bmatrix} \cos \delta & \sin \delta \\ -\sin \delta & \cos \delta \end{bmatrix}$$

with

$$\cos \delta \approx 1$$

$$\sin \delta \approx \delta \approx \frac{1}{2}(e_{xy} - e_{yx})$$

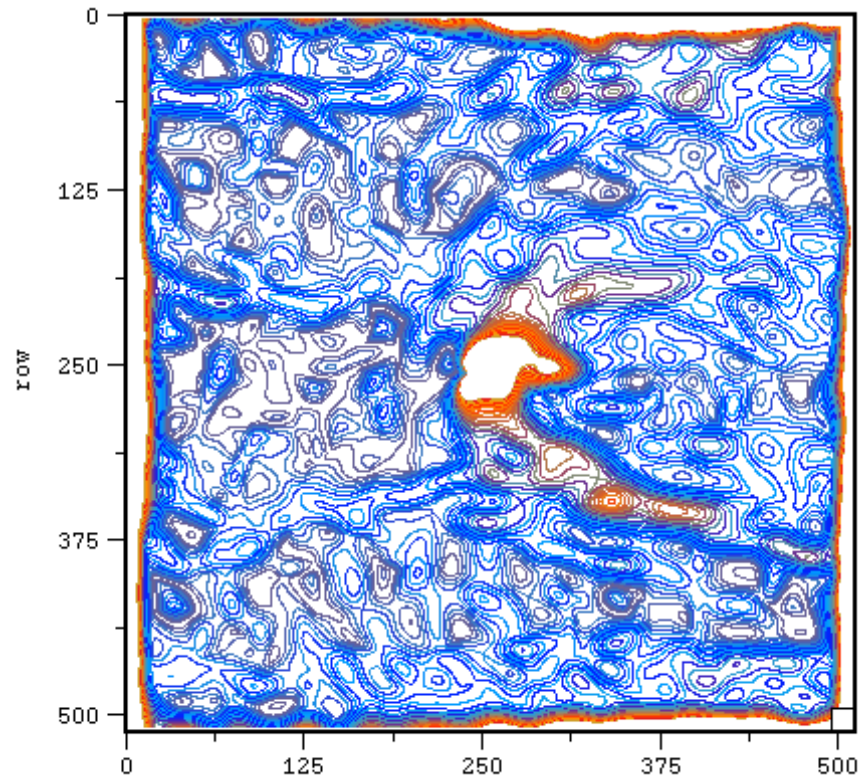
Thus we have the symmetric strain matrix

$$e' = \begin{bmatrix} e'_{xx} & e'_{xy} \\ e'_{yx} & e'_{yy} \end{bmatrix}$$

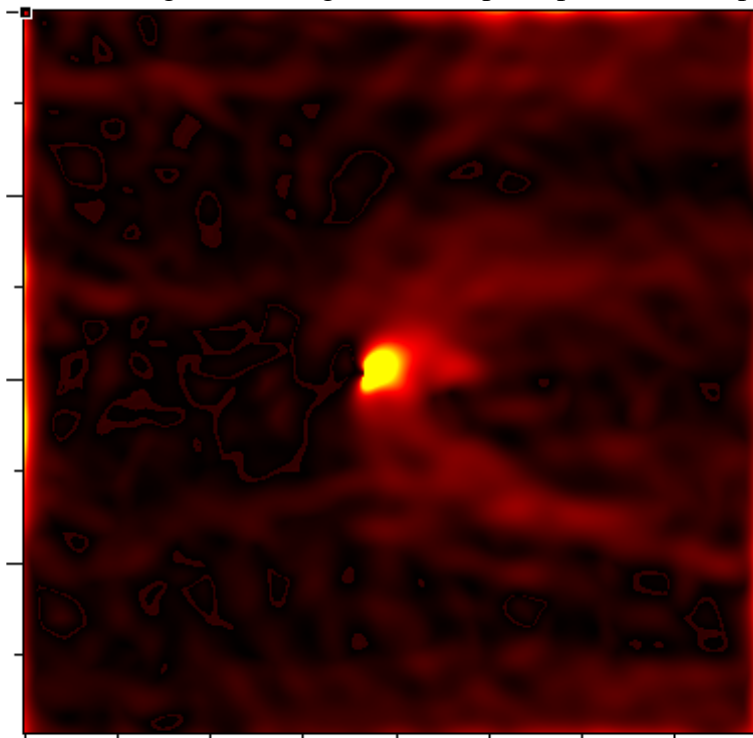
which is calculated and the three components are shown as images.

The strain can also be represented as two principal strain components along the principal strain directions. The two components are represented as the two vectors \mathbf{e}_1 and \mathbf{e}_2 . These are also calculated and the images e_{1x}, e_{1y} and e_{2x} and e_{2y} are displayed. These are the x,y components of the two principal strain vectors respectively.

Contour map of the magnitude of one of the principal strain components.



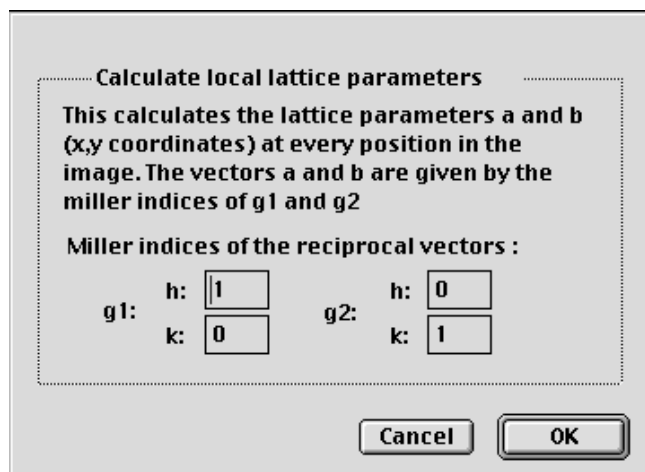
Pseudo colored image of the magnitude of a principal strain component.



Calculate Local Lattice

Calculate Local Lattice

This command is used to calculate the local lattice parameters a and b at different points in the image. It uses the local values for \mathbf{g}_1 and \mathbf{g}_2 at each point together with the Miller indices of the two reflections to refer to a lattice given by the vectors \mathbf{a} and \mathbf{b} . Not that the y-coordinate can either refer to picture coordinates (0,0 top left) or a normal coordinate system (x,y) depending on what is set under Preferences.

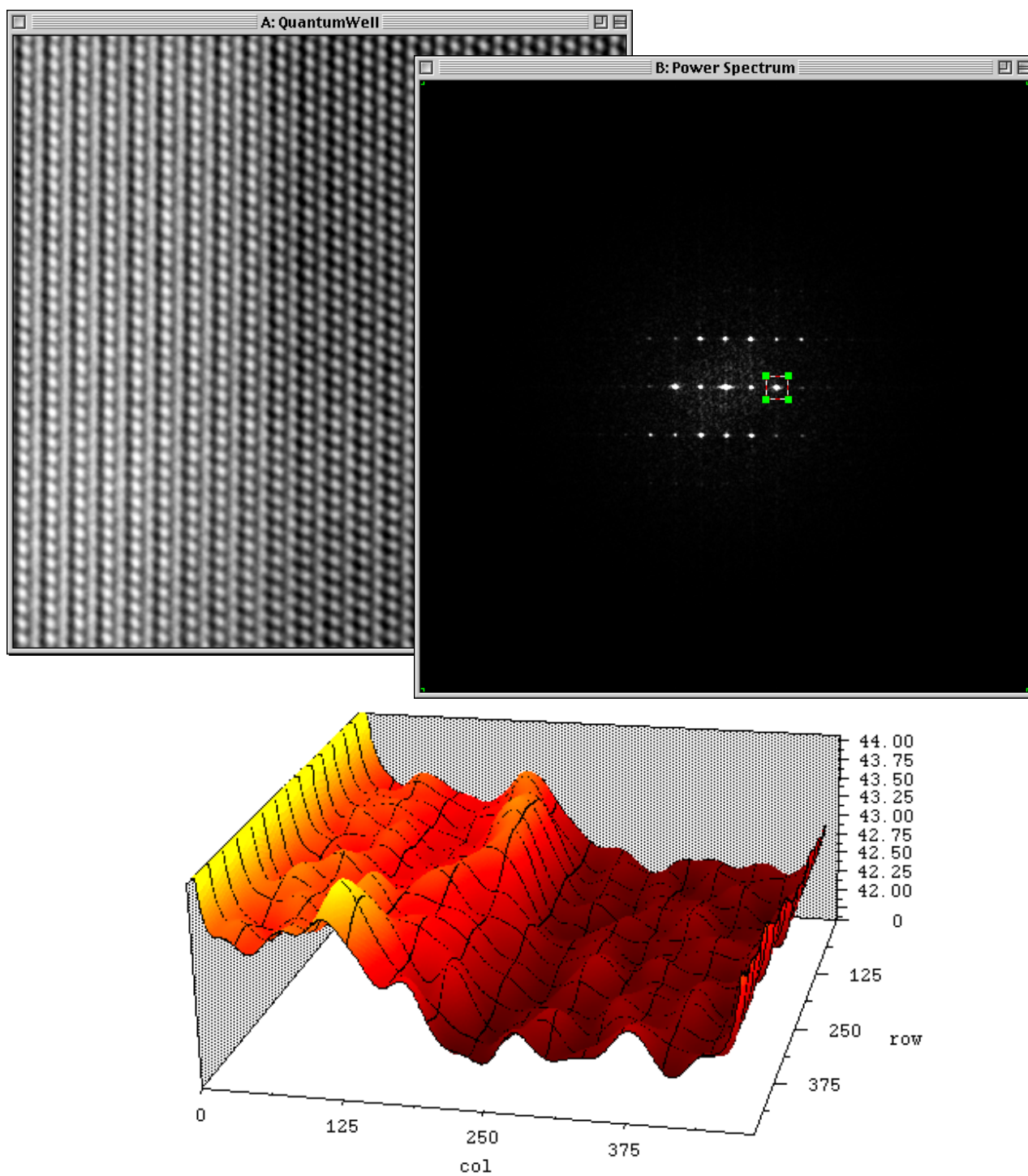


Prerequisite:

Both vectors \mathbf{g}_1 and \mathbf{g}_2 together with the respective phase images Phase Image 1 and Phase Image 2 must have been set.

Example

The images shown on the next page illustrate the use of the routine on a HRTEM image of a quantum well in In(Ga)N. Left image is the HRTEM image and the right image shows the power spectrum and one of the reflections used for calculating the lattice. The third image at the bottom is a surface plot of the a -lattice parameter as a function of position in the image.



Unwrap Phase (x,y)

Unwrap Phase (x,y)

The command “Unwrap Phase(x,y)” will try to unwrap the phase in the image “Phase Image”.

The user is prompted for a starting position which is assigned the phase at that point. The routine then moves first along each row, trying to preserve continuity in the phase value. Instead of making a jump from $\pi-\partial$ to $-\pi+\partial$, the phase will take on the value $\pi+\partial$ and continue to increase or decrease when crossing phase jumps.

This command first does the rows and then the columns of the image.

Unwrap Phase (y,x)

Unwrap Phase (y,x)

The command “Unwrap Phase(y,x)” will try to unwrap the phase in the image “Phase Image”.

The user is prompted for a starting position which is assigned the phase at that point. The routine then moves first along each column, trying to preserve continuity in the phase value. Instead of making a jump from $\pi-\partial$ to $-\pi+\partial$, the phase will take on the value $\pi+\partial$ and continue to increase or decrease when crossing phase jumps.

This command first does the columns and then the rows of the image.

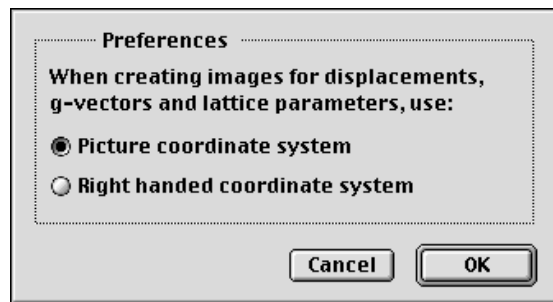
Preferences

Preferences

When the routines refer to x and y components of either reciprocal lattice vectors \mathbf{g}_1 , \mathbf{g}_2 , lattice parameters \mathbf{a} , \mathbf{b} or displacements, there is a choice in the direction of the y-axis. Normally image display programs refer to x,y being (0,0) at the top left corner of the image with y increasing downwards, while many users prefer to think of a right handed coordinate system with y

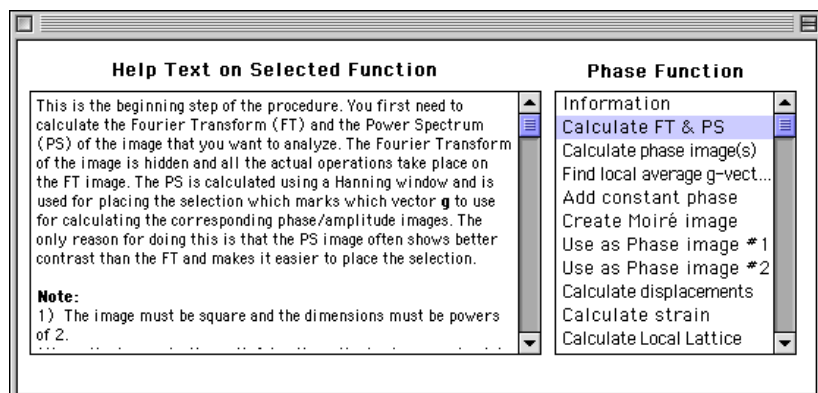
increasing up and the z-axis pointing towards the observer. When the program refers to the vectors **g** as they are reported in the Result window of Digital Micrograph, it uses a right handed coordinate system. However when images are created to hold values for the components of the displacement, lattice parameters and reciprocal lattice parameters, it is often more convenient to refer to the y-component in the picture coordinate system.

Thus depending on how the data is used, the choice of coordinate system can be changed by the user.



Help

Help



Help produces a window which allows you to access the information in this manual from within the program.